Physical characteristics of an exciton confined in a GaAs/AlGaAs single quantum well structure

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In this work we have investigated the variational parameters of a trial wave function which usually apply for investigation of excition properties in GaAs/AlGaAs quantum well structure. The interval of variation and physical meaning of these free parameters have been discussed. The tunneling behavior of an electron and hole and some other their physical properties have investigated.

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1. Introduction

Since the first semiconductor heterostructures were fabricated, the study of exciton properties, influenced by effective mass mismatch, have attracted great amount of interests especially for heterostructures based on III–V semiconductor [1–4]. Although these studies include a vast portion of the exciton properties like, localization effects [5-6], Exciton formation [7-8], exciton recombination [9], exciton dressing [10] and some others, but there is not a work about some physical properties of the excitons which we have discussed here.

In this study, by using a Monte Carlo method, we have extracted variational parameters of a trial wave function have usually been used in excition investigations, then the binding energy of an exciton confined in a $GaAs_{(1-x)}Al_x/GaAs$ single quantum well is calculated. In this work we have only investigated the binding energy of heavy hole excitons. It is usual to attribute some dimensionality character to the variational parameters of some typical trial wave functions. In the literatures [11] some deterministic behaviors are presented for these parameters. In this study we have found a stochastic behavior for these parameters. Then a conclusion is that attributing any mining to such variational parameters is meaningless. In additions we have investigated the electron and holes subband energies, tunneling effects for electron and hole and some others which are more described in the following sections.

2. Formalism

The Hamiltonian governs on the behavior of an exciton confined in a single quantum well structure, in the cylindrical coordinate have the following form [12],

$$H=\sum_{i=e,h}\left(-\frac{\hbar^2}{2m_i}\frac{\partial^2}{\partial z_i^2}+V_i^{conf}(z_i)\right)-\frac{\hbar^2}{2\mu}\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}-\frac{e^2}{\varepsilon_0\sqrt{\rho^2+(z_e-z_h)^2}} \quad (1)$$

where $\frac{1}{\mu_\pm}=\frac{1}{m_e}+\frac{(\gamma_1\pm\gamma_2)}{m_0}$ is the reduced mass corresponding to the heavy (+) and light hole (-), $m_{h\pm}^z=\frac{m_0}{\gamma_1\mp 2\gamma_2}$, $m_h^\perp=\frac{m_0}{\gamma_1+\gamma_2}$ are the heavy hole effective mass along the z direction and in the plane perpendicular to it [13], $\rho=\rho_e-\rho_h$ is the relative coordinate and γ_1 and γ_2 are the Kohn–Luttinger band parameters which are the same as those of used in work of Senger et al. These parameters and are presented in the Table 1. There are different methods in order to extract the variational parameters of the trial wave functions or to find the E_0 by using equation (16). Differentiation with respect to the variational parameters and equating to zero is a way for this purpose. Plotting the energy as a function of the variational parameters in a multidimensional space [14] or using stochastic methods like Monte Carlo [15] and genetic algorithms [16] are other methods which may be used. In this work we have used Monte Carlo schema. In the literatures there are different types of trial wave functions for a confined exciton in quantum wells. The most frequently used trial wave function has been used by Senger et al [12]:

$$\psi(\vec{r}_e,\vec{r}_h)=f_e(z_e)f_h(z_h)\exp(-\lambda\sqrt{\rho^2+a^2(z_e-z_h)^2})\times\exp(-b^2\rho^2) \quad (2)$$

where λ, a and b are the free parameters of this trial wave function and $f_i(z_{i=e,h})$ are the envelop functions which reads:

$$f_{e,h}(z_{e,h}) = \begin{cases} \cos(k_{e,h} z_{e,h}), & |z_{e,h}| < L/2 \\ A_{e,h} e^{-K_{e,h}|z_{e,h}|}, & |z_{e,h}| > L/2 \end{cases} \quad (3)$$

where e and h indicate the electron and hole. λ, a and b are the free parameters of this trial wave function. Now the ground state energy can be found by the minimization of $E_0 = Min_{a,b,\lambda} \langle \psi | H | \psi \rangle$.

Table 1. Material parameters for the $Al_{(1-x)}Ga_xAs/GaAs$.

Material	m_e	γ_1	γ_2	ε_0	reference
GaAs	0.067	6.98	2.06	12.5	[22]
$Al_{0.3}Ga_{0.7}As$	0.067	6.93	2.15	12.5	[22]

3. Results and discussion

The exciton binding energy is written as $E_b=E_g + E_e + E_h - E_{ex}$ where E_g, E_e and E_h are energy gap and subband energies respectively. E_{ex} is defined as the energy eigenvalue of the Hamiltonian in equation (1). The subband energies E_e and E_h may found by using these equations:

$$\left[\frac{E_e}{V_e}\right]^{1/2} = \cos\left[\left[\frac{m_e E_e}{2\hbar^2}\right]^{1/2} L\right], \quad \left[\frac{E_h}{V_h}\right]^{1/2} = \cos\left[\left[\frac{m_h E_h}{2\hbar^2}\right]^{1/2} L\right] \quad (4)$$

These equations can be solved by bisection method [17]. This result is shown in the Fig. 1. As one expects the energies decrease when the well width increases and we approach the bulk limit. In order to include the effect of the effective mass mismatch in the well and barrier we have used the Ben-Daniel-Duke boundary condition [18]. The effective mass of the electron and hole in the well has also been obtained by the Vegard law [19]. We have used the material parameters as follows [20]. The total energy band gap difference $\Delta E_g(x)$ between GaAs and $Al_xGa_{1-x}As$ is $\Delta E_g = 1.155x + 0.37x^2$(ev). If we show the conduction and valance band offsets as of v_e^0 and v_h^0 respectively then we have $v_e^0 = AE_g \times C$ and $v_h^0 = AE_g \times (1-C)$ where C a positive value. Other physical constant are given in the Table 1.

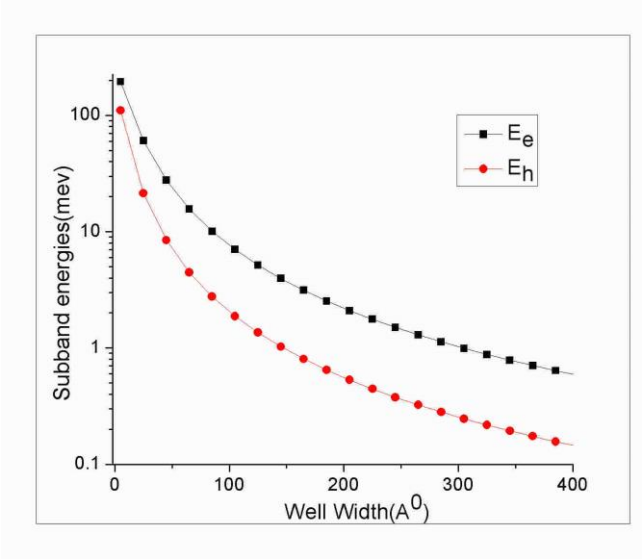

Fig. 1. Variation of the subband energies E_e an E_h as a function of well width.

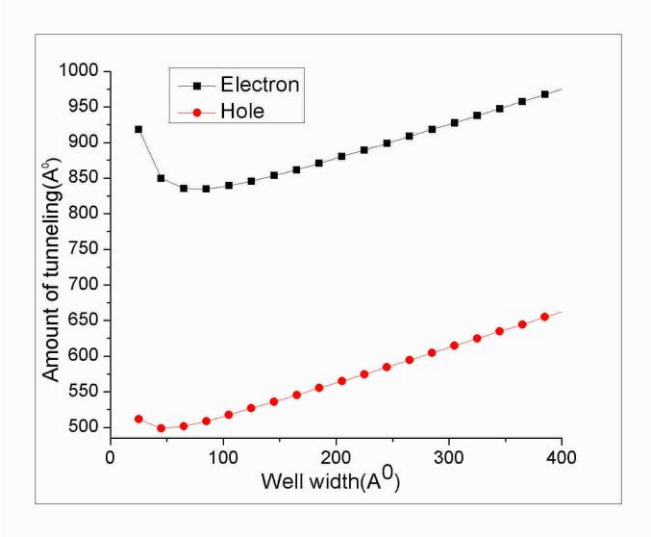

Fig. 2. Amount of tunneling of electron and hole as a function of the well width.

In order to perform the integrations numerically we have to assume a finite value for limits of the integration along growth direction for electron and hole (z_e and z_h). We have selected the integral limits as the points where the wave function fall down by some percent of its value at the interface of the well and barrier. By this method, we have estimated the amount of tunneling of electrons and holes into the barriers. The result is presented in the Fig. 3. We have obtained the amount of tunneling as the distance where the wave function (in the barriers) reduces up to 10^{-6} times of its maximum value at the interface. As we can see in the Fig. 3, there is a non-monotonic change in the variation of the tunneling of the electron and hole into the barrier due to the non-monotonic behavior of the two dimensional Coulomb interactions as a function of the well width. As one may expect the amount of electrons

tunneling (with smaller effective mass) is greater than the amount of holes tunneling but the style of the variation is the same for both of electrons and holes. We have used the same number of the Monte Carlo sampling points for all the well widths. The variation of the wave numbers ($K_{e,h}$ $k_{e,h}$) and amplitudes $A_{e,h}$ as a function of the well width which are presented in the Figs. 4 and 5 respectively. $A_{e,h}$ is proportional to probability of finding the electrons in the barrier regions.

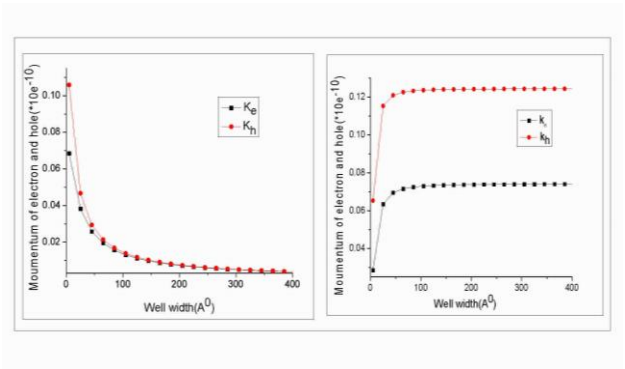

Fig. 3. Variation of the momentums $K_{e,h}$, $k_{e,h}$ as a function of the well width.

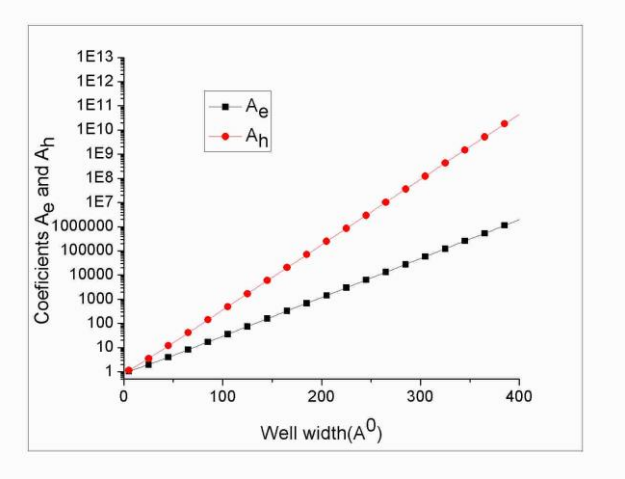

Fig. 4. Variation of the coefficients $A_{e,h}$ as a function of the well width.

Now we have used some trial wave functions and tried to find the exciton binding energy. We have calculated the exciton binding energy by using of the equations (2), with different values for its parameters. The results have been shown in the Fig. 5. For comparison we have also plotted the exciton binding energy taken from the ref [13, 22]. As the figure shows, if we use the trial wave function with $a \in [0,1] \,\&\, \lambda \in [0,10^8]$ the consistency between our calculated exciton binding energy and the results of the other groups have shown in the ref [13, 22] is not good. When we apply $a \in [0,10^4] \,\&\, \lambda \in [0,10^4]$ or $a,b,\lambda \in [0,10^3]$ there is better agreement with the ref [13,22]. In this calculation we have used smaller upper bound for the free parameters a, b, λ. If we choose two or three of these parameters in a larger interval, e.g. $a,b,\lambda \in [0,10^8]$, this always leads to a zero trial wave function. The small oscillatory behavior is due to the stochastic nature of the Monte Carlo method we have applied. In order to reduce such oscillation we have used the averaging technique. We have used 15 times averaging to find our results.

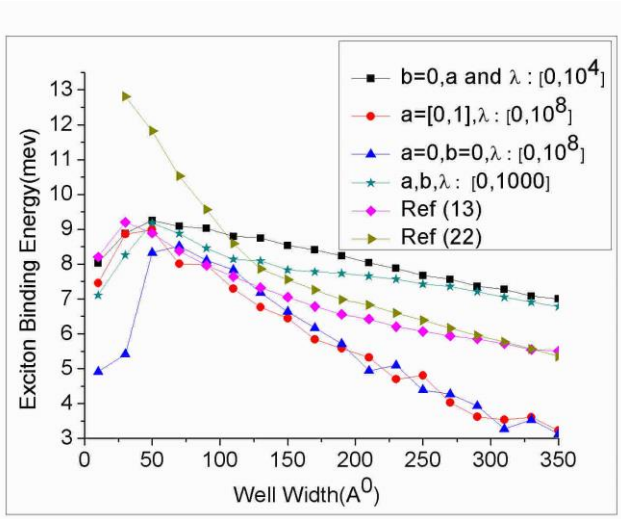

Fig. 5. Variation of the exciton binding energy as a function of well width for different types of the trial wave functions and different interval for the free parameters. For comparison the exciton binding energy obtained by the ref [13,22] is also presented.

In the Fig. 6, we have presented the behavior of different variational parameters which were introduced in equations (2). In the Fig. (6-a) variation of λ as a function of the well width is shown. In the inset of this figure the variation of the exciton Bohr radius ($1/\lambda$) versus the well width is also depicted. This behavior is not completely the same as that of obtained by Harrison et al. [21]. This is partially due to the computational inaccuracy. This trial wave function works correctly in the two dimensional limit and it can also be used it in the three dimensional limit in order to find the bulk exciton binding energy. This is the power of the variational method which by using a completely arbitrary trial wave function a good accuracy may be achieved. In the Fig. (6-b) variation of the free parameters a, b, $\lambda \in [0,10^3]$ of the trial wave function defined by the equation (2) is shown. These parameters do not show any regular mode of variation. In the Figs. 6-a and 6-b free parameters of the equation (2) are evaluated. As it is well-known [21] variation of the parameters 'a' and λ at b=0 has a regular form. It is also better that the values of the 'a' parameter to be in the range of [0, 1]. When we allowed the parameters 'a' and λ to vary within the regions [0, 1] and [0, 10^8] respectively we do not find the same variation as that has reported in the ref [21]. Then we allowed the 'a' and λ to vary in the range of [0, 10^4].

The result is shown in the Fig. 6-d. By this selection the variations, the calculated exciton binding energy, (Figs. 5), has a good accuracy despite the fact that the variations of the free parameters do not have regular behavior. Harrison et al. were related a dimensionality character to the variational parameters of this trial wave function [21] but our calculations (6-c) and (6-d) show that these parameters do not behave in a manner that one be able to assign such meaning to them. In fact these are only some free parameters which may be obtained by different manners and within various ranges.

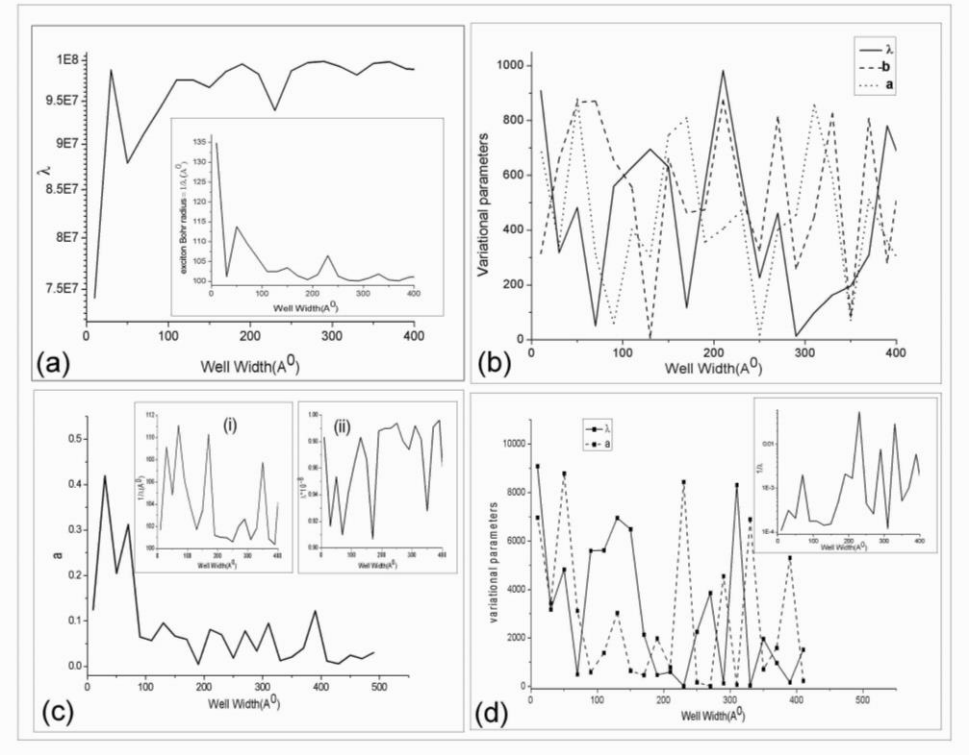

Fig. 6. Variation of the trial wave functions free parameters used in this work as a function of well width. (a) Variation of the free parameters λ in for equation (2) for (a=b=0) and its inverse (exciton bohr radius). (b) Free parameters of the equation (2) with the range of variation [0, 1000]. (c) Parameter 'a' in equation (2) for (b=0) with the range of variation [0-1]. In the insets variation of the free parameter λ with the range of variation [0, 1] and its inverse as a function of the well with is plotted. (d) Parameter 'a' in equation (2) for (b=0) with the range of variation [0, 10^8]. In the insets variation of the inverse of the free parameter λ as a function of the well with is presented.

4. Conclusion

In this work, we have investigated some aspects of excitons confined in a GaAs/AlGaAs single quantum well structure. The most important results of this study are as follows. There is a non-monotonic change in the variation of the tunneling of the electron and hole into the barrier. The amount of electrons tunneling is greater than the amount of holes tunneling in the barrier. In the Harrison et al. work, some variational parameters of the trial wave function in equation (2) are obtained by a non-stochastic method, thus they found them to vary in a non-stochastic behavior. Then they assigned a dimensionality character to the mentioned variational parameters. But our calculations based on a stochastic method (Monte Carlo) showed that these parameters do not behave in a straightforward manner thus one is not able to assign a meaning to them since the physics of the problem should not change by changing the method of calculation. However, since these variational parameters can have different values based on the method of calculations thus we can not assign a physical meaning like dimensionality character to them

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